CSC

Elmer Software Development Practices APIs for Solver and UDF

ElmerTeam CSC – IT Center for Science

CSC, November.2015

Elmer programming languages

- Fortran90 (and newer)
 - ElmerSolver (~240,000 lines of which ~50% in DLLs)

C++

- ElmerGUI (~18,000 lines)
- ElmerSolver (~10,000 lines)

C

- ElmerPost (~45,000 lines)
- ElmerGrid (~30,000 lines)
- MATC (~11,000 lines)



Tools for Elmer development

- Programming languages
 - Fortran90 (and newer), C, C++
- Compilation
 - Compiler (e.g. gnu), configure, automake, make, (cmake)
- Editing
 - emacs, vi, notepad++,...
- Code hosting (git)
 - Current: https://github.com/ElmerCSC
 - Obsolite: www.sf.net/projects/elmerfem
- Consistency tests
- Code documentation
 - Doxygen
- Theory documentation
 - Latex
- Community server
 - www.elmerfem.org (forum, wiki, etc.)



Elmer libraries



- Required: Matc, Hutlter, Lapack, Blas, Umfpack (GPL)
- Optional: Arpack, Mumps, Hypre, Pardiso, Trilinos,
 SuperLU, Cholmod, NetCDF, HDF5, ...
- ElmerGUI
 - Required: Qt, ElmerGrid, Netgen
 - Optional: Tetgen, OpenCASCADE, VTK, QVT



Elmer licenses



- ElmerSolver library is published under LGPL
 - Enables linking with all license types
 - It is possible to make a new solver even under proprietary license
 - Note: some optional libraries may constrain this freedom due to use of GPL licences
- Rest of Elmer is published under GPL
 - Derived work must also be under same license ("copyleft")

Elmer version control at GitHub

In 2015 the official version control of Elmer was transferred from svn at sf.net to git hosted at GitHub

- Git offers more flexibility over svn
 - Distributed version control system
 - Easier to maintain several development branches
 - More options and hence also steeper learning curve
 - Developed by Linus Torvalds to host Linux kernel development
- GitHub is a portal providing Git and some additional services
 - Management of user rights
 - Controlling pull requests

Git- Version control system

- Elmer uses git version control system for the code repository and development
 - Hosted at github
 - Development version in "trunk" is considered stable
 - To obtain the whole source code

git clone https://github.com/ElmerCSC/elmerfem.git

- Git client available in command line in *nix systems
- In Windows systems a nice graphical client is "Tortoise"

Elmer at Github

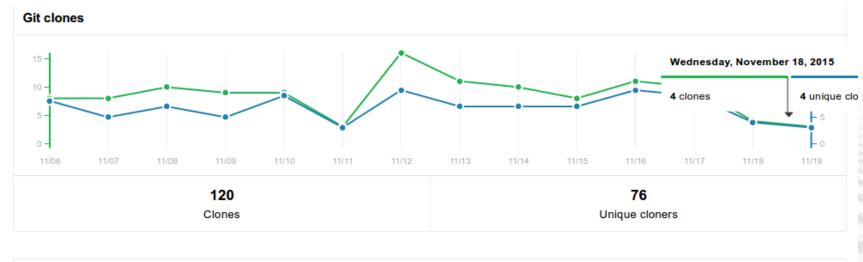
https://github.com/ElmerCSC

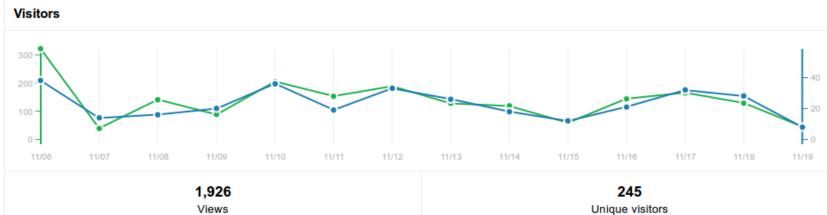
GitHub Search GitHub	Explore Features Enterprise	Pricing Sig	gn up Sign in
Elmer developer team The http://elmerfem.org/ Image elmeradm@csc.fi Repositories			
Filters - Q Find a repository		People	0 >
elmerfem Official git repository of Elmer FEM software Updated a minute ago	FORTRAN ★ 43 🎾 19	This organization has no You must be a member t of this organi	o see who's a part
opuated a minute ago			
homebrew-elmerfem Homebrew formula for installing Elmer on Macs Updated on 31 Aug	Ruby 🛨 0 😢 0		

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Activity on Github







Elmer is published under (L)GPL

- Used worldwide by thousands of researchers (?)
- One of the most popular open source multiphysical software

Count	try / Territory	Visits 🗸	Pages / Visit	Avg. Visit Duration	% New Visits	Bounce Rate
1.	United States	9,611	3.52	00:03:31	55.59%	60.55%
2.	Germany	8,938	5.08	00:05:52	31.76%	51.92%
3.	France	4,404	3.15	00:03:06	30.68%	68.66%
4.	United Kingdom	4,028	4.19	00:04:27	39.03%	53.87%
5.	Finland	3,841	7.06	00:09:14	20.57%	22.49%
6.	Italy	3,602	4.44	00:03:38	55.19%	47.47%
7.	Spain	1,957	6.16	00:05:52	36.54%	46.65%
8.	Japan	1,484	3.14	00:03:20	36.59%	64.08%
9.	India	1,341	2.86	00:02:39	73.38%	69.57%
10.	Canada	1,335	3.12	00:02:53	58.13%	63.00%
11.	Netherlands	1,333	3.73	00:03:44	37.21%	58.21%
12.	Austria	1,120	4.88	00:04:43	29.29%	53.04%
13.	Switzerland	995	3.63	00:03:23	40.80%	59.30%
14.	China	975	4.14	00:04:04	48.92%	53.54%
15.	Poland	907	4.06	00:03:59	41.23%	55.35%
16.	Brazil	876	2.98	00:03:16	42.01%	64.50%
17.	Russia	831	2.97	00:02:53	51.50%	65.82%

~20k Windows downloads at sf.net in a year

Home / WindowsBinaries (Change File)

Date Range: 2012-04-01 to 2013-03-31

DOWNLOADS

19 185

In the selected date range

TOP COUNTRY

United States

16% of downloaders

TOP OS

Windows

93% of downloaders

OS downloads as: Percent

	Country +	Android +	BSD +	Linux +	Macintosh +	Unknown +	Windows +	Total •
1.	United States	0%	0%	3%	3%	1%	80%	3,182
2.	Germany	0%	0%	4%	1%	0%	80%	2,313
3.	Italy	0%	0%	3%	1%	0%	80%	1,537
4.	France	0%	0%	4%	1%	1%	79%	798
5.	India	0%	0%	6%	1%	4%	78%	782
6.	Russia	0%	0%	4%	0%	0%	77%	772
7.	United Kingdom	0%	0%	3%	2%	0%	81%	642
8.	China	0%	0%	3%	1%	1%	78%	637
9.	Japan	0%	0%	2%	2%	0%	77%	599
10.	Spain	0%	0%	6%	0%	20%	63%	561
11.	Poland	0%	0%	2%	0%	0%	87%	532
12.	Canada	1%	0%	2%	2%	0%	85%	410
13.	Brazil	0%	0%	4%	1%	0%	88%	391
14.	Finland	0%	0%	2%	1%	0%	78%	300

16k Windows downloads at sf.net in a year



	Country +	Downloads A
1.	United States	2,553
2.	Germany	2,529
3.	Italy	1,342
4.	Russia	975
5.	Japan	789
6.	United Kingdom	609
7.	France	548
8.	China	529
9.	India	483
10.	Spain	400
11.	Poland	385
12.	Finland	305

Installers

- Fresh Windows installers
 - Currently only 64 bit version
 - Also a parallel version with msmpi
 - http://www.nic.funet.fi/pub/sci/physics/elmer/bin/windows/
- Elmer for Debian & Ubuntu etc. at launchpad
 - Nightly builds from Git repository
 - To install
 - \$ sudo apt-add-repository ppa:juhmat/elmer-test
 - \$ sudo apt-get update
 - \$ sudo apt-get install elmerfem-csc



Cmake build system



- During 2014-2015 Elmer was migrated from gnu autotools to cmake
- cmake offers several advantages
 - Enables cross compilation for different platforms (e.g. Intel MICs)
 - More standardizes installation scripts
 - Straight-forward package creation for many systems (using cpack)
 - Great testing utility with ctest
- Transition to cmake required significant code changes
 - ISO C-bindings & many changes in APIs
 - Backward compatibility in compilation lost

Obtaining the source code

- To clone the code (this is anonymously): git clone \ https://github.com/ElmerCSC/elmerfem.git
 - We work with branches. To change into another branch:

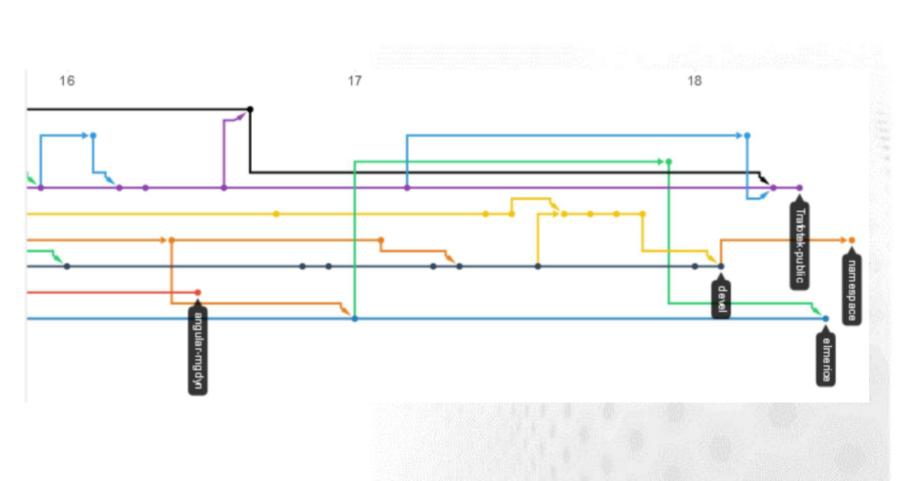
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cd elmerfem

git checkout branchname

- We use the following branches (confined to most important):
 - release: contains stable release (~half-yearly update)
 - *devel*: our main branch from which you should get latest updates
 - *elmerice*: the main developer branch for Elmer/Ice
 NB: you might have to do a

git checkout --track origin/elmerice



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Obtaining the source code

On branches:

Code organization

Source of ElmerSolver
MATC language
Fortran version of linear algebra solvers
Graphical User Interface t Elmer based on QT4
Elmer/Ice solver and function source code
Legacy visualization tool
Grid manipulation for Elm
Contains Lapack/BLAS fro netlib (avoid using them)
Additional package for optimization



Compilation of the whole code with cmake



To compile the whole code see example scripts under

www.csc.fi/elmer and www.elmerfem.org

```
ELMERSRC="/path/to/sourcecode/elmerfem"
BUILDDIR="/path/too/existing/and/empty/builddir"
IDIR="/path/to/installation/dir/"
TOOLCHAIN="/path/to/optional/toolchainfile.smake"
cmake $ELMERSRC \
    -DCMAKE BUILD TYPE=DEBUG\
    -DCMAKE INSTALL PREFIX=$IDIR \
    -DWITH MPI:BOOL=TRUE \
    -DWITH Mumps: BOOL=TRUE \
    -DWITH Hypre:BOOL=TRUE \
    -DWITH ELMERGUI: BOOL=TRUE \
    -DWITH OCC:BOOL=TRUE \
    -DWITH PARAVIEW: BOOL=TRUE \
    -DWITH PYTHONOT: BOOL=TRUE \
    -DWITH QWT:BOOL=TRUE \
    -DWITH VTK:BOOL=TRUE \
    -DWITH PYTHONQT:BOOL=FALSE \
    -DWITH MATC:BOOL=TRUE \
    -DWITH ElmerIce: BOOL=TRUE
```

Consistency tests



- Simple shell script to run through the cases + piece of C-code to compare the norm of solutions
- There are >300 consistency tests (November 2015)
 - Located under fem/tests, run with ctest in build-directory
- Each time a significant commit is made the tests are run with the fresh version
 - Aim: trunk version is a stable version
 - New tests for each major new feature
- The consistency tests provide a good starting point for taking some Solver into use
 - cut-paste from sif file
- Note: the consistency tests have often poor time and space resolution for rapid execution

Consistency tests - example

Terminal		- + ¥
zwinger@elmeruser-VM64bit ~/Source/Elmer devel/elmerfem \$ co		~
zwinger@elmeruser-VM64bit ~/Source/Elmer devel \$ cd builddin		,
zwinger@elmeruser-VM64bit ~/Source/Elmer_devel/builddir_elme	_	
erice		
Test project /home/zwinger/Source/Elmer devel/builddir elmer	ice	
Start 35: mgdyn lamstack widefreg harmonic		
1/379 Test #35: mgdyn lamstack widefreg harmonic	Passed	12.58 sec
Start 36: NaturalConvectionRestart		
2/379 Test #36: NaturalConvectionRestart	Passed	10.90 sec
Start 37: ContactPatch3D		
3/379 Test #37: ContactPatch3D	Passed	4.28 sec
Start 38: ContactPatch3D_np4		
4/379 Test #38: ContactPatch3D_np4	Passed	6.13 sec
Start 39: CurvedBndryPFEM		
5/379 Test #39: CurvedBndryPFEM	Passed	0.12 sec
Start 40: heateq		
6/379 Test #40: heateq	Passed	0.42 sec
Start 41: StrainCalculation02		
7/379 Test #41: StrainCalculation02	Passed	8.62 sec
Start 42: ContactPatch2Dtwo		
8/379 Test #42: ContactPatch2Dtwo	Passed	0.16 sec
Start 43: freesurf	Desert	1 (1
9/379 Test #43: freesurf	Passed	1.61 sec
Start 44: rotflow		

Doxygen – WWW documentation

🕹 Elmer finite eleme	ent software: Modules - M	lozilla Firefox	and the second			- 0 X
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Done						a

Doxygen – Example in code



Special comment indicators: !> and <!</p>

```
|______
!> Subroutine for computing fluxes and gradients of scalar fields.
!> For example, one may compute the the heat flux as the negative gradient of temperature
!> field multiplied by the heat conductivity.
!> \ingroup Solvers
1-----
SUBROUTINE FluxSolver( Model, Solver, dt, Transient )
USE CoordinateSystems
USE DefUtils
IMPLICIT NONE
TYPE (Solver t) :: Solver !< Linear & nonlinear equation solver options
TYPE(Model_t) :: Model !< All model information (mesh, materials, BCs, etc...)</pre>
LOGICAL :: Transient !< Steady state or transient simulation
_____
  Local variables
 _____
TYPE (ValueList t), POINTER :: SolverParams
```



Doxygen – Example in WWW



subroutine FluxSolver (TYPE(Model_t)	Model,
	TYPE(Solver_t)	Solver,
	REAL(KIND=dp)	dt,
	LOGICAL	Transient
)		

Subroutine for computing fluxes and gradients of scalar fields. For example, one may compute the the heat flux as the negative gradient of temperature field multiplied by the heat conductivity.

Parameters:	
Solver	Linear & nonlinear equation solver options
Model	All model information (mesh, materials, BCs, etc)
dt	Timestep size for time dependent simulations
Transient	Steady state or transient simulation

References BulkAssembly().

Here is the call graph for this function:



Compilation of a DLL module

Applies both to Solvers and User Defined Functions (UDF)

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- Assumes that there is a working compile environment that provides "elmerf90" script
 - Comes with the Windows installer, and Linux packages
 - Generated automatically when ElmerSolver is compiled

elmerf90 MySolver.f90 -o MySolver.so

User defined function API

```
_____
!> Standard API for UDF
           _____
RECURSIVE FUNCTION MyProperty (Model, n, t) RESULT(f)
 _____
 USE DefUtils
 IMPLICIT NONE
         _____
 TYPE (Model t) :: Model !< Handle to all data
 INTEGER :: n
                    !< Current node
 REAL(KIND=dp) :: t
                     !< Parameter(s)</pre>
 REAL(KIND=dp) :: f
                    !< Parameter value at node</pre>
```

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Actual code ...

Function API



MyProperty = Variable time
"MyModule" "MyProperty"

- User defined function (UDF) typically returns a real valued property at a given point
- It can be located in any section that is used to fetch these values from a list
 - Boundary Condition, Initial Condition, Material,...

Solver API



```
_____
!> Standard API for Solver
           _____
SUBROUTINE MySolver( Model,Solver,dt,Transient )
 USE DefUtils
 IMPLICIT NONE
         _____6888
 TYPE(Solver t) :: Solver !< Current solver
 TYPE (Model t) :: Model !< Handle to all data
 REAL(KIND=dp) :: dt !< Timestep size
 LOGICAL :: Transient
                   !< Time-dependent or not
```

Actual code ...

Solver API



```
Solver 1
  Equation = "MySolver"
  Procedure = "MyModule" "MySolver"
```

End

- Solver is typically a FEM implementation of a physical equation (PDE)
- But it could also be an auxiliary solver that does something completely different
- Solver is usually called once for each coupled system iteration

Elmer – High level abstractions

The quite good success of Elmer as a multi-physics code may be addressed to certain design choices

- Solver is an abstract dynamically loaded object
- Parameter value is an abstract property fetched from a list
- The abstractions mean that new solvers may be implemented without much need to touch the main library
 - Minimizes need of central planning
 - Several applications fields may live their life quite independently (electromagnetics and glaciology)
- MATC a poor man's Matlab adds to flexibility as algebraic expressions may be evaluated on-the-fly

Solver as an abstract object

- Solver is a dynamically loaded object (.dll or .so)
 - May be developed and compiled separately
- Solver utilizes heavily common library utilities
 - Most common ones have interfaces in DefUtils
- Any solver has a handle to all of the data
- Typically a solver solves a weak form of a differential equation

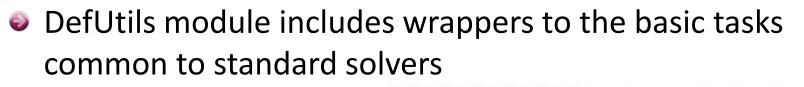
- Currently ~50 different Solvers, roughly half presenting physical phenomena
 - No upper limit to the number of Solvers
- Solvers may be active in different domains, and even meshes
- The menu structure of each solver in ElmerGUI may be defined by an .xml file

Properties as abstract objects

- Properties are saved in a list structure by their name
- Namespace of properties is not fixed, they may be introduced in the command file
 - E.g. "MyProperty = Real 1.23" adds a property "MyProperty" to a list structure related to the solver block

- In the code parameters are fetched from the list
 - E.g. "val = GetReal (Material, 'MyProperty', Found)" retrieves the above value 1.23 from the list
- A "Real" property may be any of the following
 - Constant value
 - Linear or cubic dependence via table of values
 - Expression given by MATC (MatLab/C-type command language)
 - User defined functions with arbitrary dependencies
 - Real vector or tensor
- As a result solvers may be weakly coupled without any *a priori* defined manner
- There is a price to pay for the generic approach but usually it is less than 10%
- SOLVER.KEYWORDS file may be used to give the types for the keywords in the command file

DefUtils

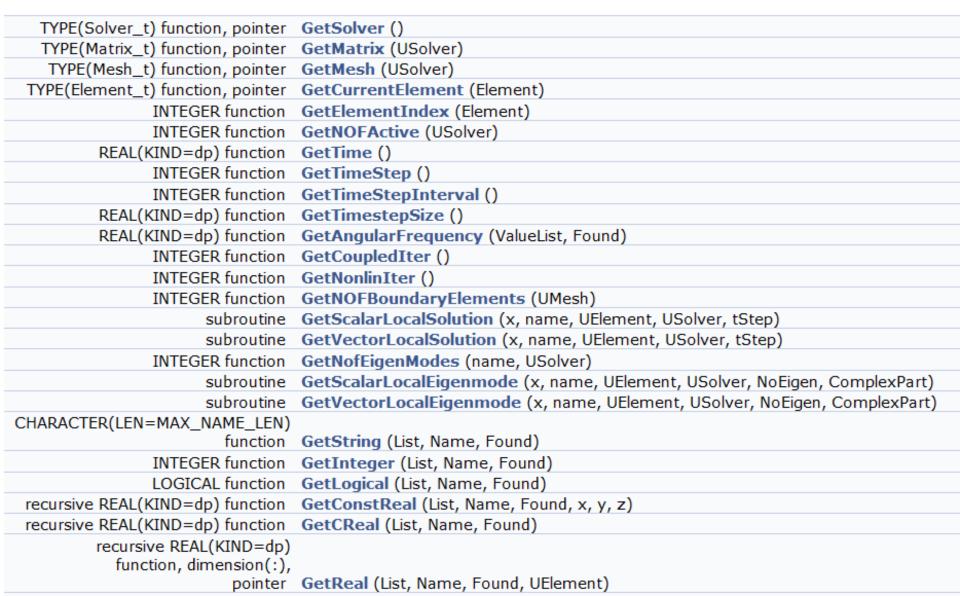


 E.g. "DefaultDirichlet()" sets Dirichlet boundary conditions to the given variable of the Solver

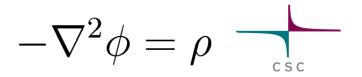
- E.g. "DefaultSolve()" solves linear systems with all available direct, iterative and multilevel solvers, both in serial and parallel
- Programming new Solvers and UDFs may usually be done without knowledge of other modules

DefUtils – some functions

Public Member Functions



Example: Poisson equation



- Implemented as an dynamically linked solver
 - Available under tests/1dtests
- Compilation by: elmerf90 Poisson.f90 -o Poisson.so
- Execution by:
 ElmerSolver case.sif
- The example is ready to go massively parallel and with all a plethora of elementtypes in 1D, 2D and 3D

Poisson equation: code Poisson.f90

!> Solve the Poisson equation -\nabla\cdot\nabla \phi = \rho
I------

SUBROUTINE PoissonSolver(Model,Solver,dt,TransientSimulation)

USE DefUtils IMPLICIT NONE

!Initialize the system and do the assembly: !-----CALL DefaultInitialize()

active = GetNOFActive() DO t=1,active Element => GetActiveElement(t) n = GetElementNOFNodes()

LOAD = 0.0d0 BodyForce => GetBodyForce() IF (ASSOCIATED(BodyForce)) & Load(1:n) = GetReal(BodyForce, 'Source', Found)

! Get element local matrix and rhs vector: !-----CALL LocalMatrix(STIFF, FORCE, LOAD, Element, n)

! Update global matrix and rhs vector from local contribs !------CALL DefaultUpdateEquations(STIFF, FORCE)

END DO

CALL DefaultFinishAssembly() CALL DefaultDirichletBCs() Norm = DefaultSolve() Solver 1 Equation = "Poisson" Variable = "Potential" Variable DOFs = 1 Procedure = "Poisson" "PoissonSolver" Linear System Solver = "Direct" Linear System Direct Method = umfpack Steady State Convergence Tolerance = 1e-09 End

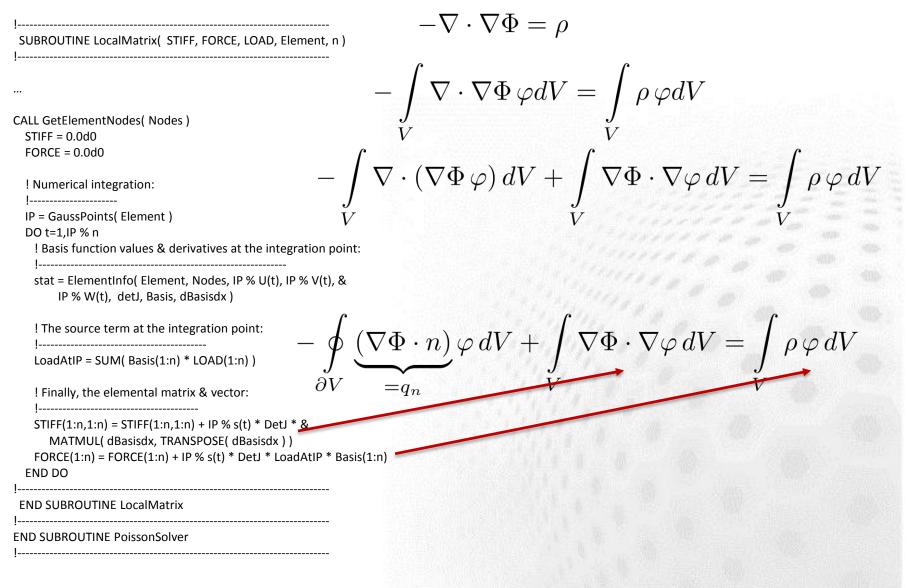
Body Force 1 Source = Variable Potential Real Procedure "Source" "Source" End

Boundary Condition 1 Target Boundaries(2) = 1 2 Potential = Real 0 End



Poisson equation: code Poisson.f90

CONTAINS



Poisson equation: source term, examples

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Constant source:

```
Source = 1.0
```

Source dependeing piecewise linear on x:

```
Source = Variable Coordinate 1

Real

0.0 0.0

1.0 3.0

2.0 4.0

End
```

Source depending on x and y:

```
Source = Variable Coordinate
Real MATC "sin(2*pi*tx(0))*cos(2*pi(tx(1))"
```

Source depending on anything

```
Source = Variable Coordinate 1
Procedure "Source" "MySource"
```

Poisson equation: ElmerGUI menus

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<?xml version='1.0' encoding='UTF-8'?> <!DOCTYPE edf> <edf version="1.0" > <PDE Name="Poisson" > <Name>Poisson</Name>

<BodyForce>

<Parameter Widget="Label" > <Name> Properties </Name> </Parameter> <Parameter Widget="Edit" > <Name> Source </Name> <Type> String </Type> <Whatis> Give the source term. </Whatis> </Parameter>

</BodyForce>

<Solver>

```
<Parameter Widget="Edit" >
```

<Name> Procedure </Name>

<DefaultValue> "Poisosn" "PoissonSolver" </DefaultValue>

</Parameter>

```
<Parameter Widget="Edit">
```

```
<Name> Variable </Name>
```

<DefaultValue> Potential</DefaultValue>

```
</Parameter>
```

</Solver>

```
<BoundaryCondition>
```

<Parameter Widget="Label" > <Name> Dirichlet conditions </Name> </Parameter>

<Parameter Widget="Edit">

<Name> Potential </Name>

<Whatis> Give potential value for this boundary. </Whatis>

</Parameter>

</BoundaryCondition>

</PDE>

</edf>

Development tools for ElmerSolver

- Basic use
 - Editor (emacs, vi, notepad++, jEdit,...)
 - elmerf90 script
- Advanced
 - Editor
 - git client
 - Compiler suite (gfortran, ifort, pathf90, pgf90,...)
 - Documentation tools (Doxygen, LaTeX)
 - Debugger (gdb)
 - Profiling tools

Elmer – some best practices

- Use version control when possible
 - If the code is left to your own local disk, you might as well not write it at all

- Never fork! (user base of 1000's)
- Always make a consistency test for a new feature
 - Always be backward compatible
 - If not, implement a warning in the code
- Maximize the level of abstraction
 - Essential for multi-physics software
 - E.g. any number of physical equations, any number of computational meshes, any number of physical or numerical parameters – without the need for recompilation